Numerical simulation of the fractional Bloch equations

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Abstract

In physics and chemistry, specifically in NMR (nuclear magnetic resonance) or MRI (magnetic resonance imaging), or ESR (electron spin resonance) the Bloch equations are a set of macroscopic equations that are used to calculate the nuclear magnetization $\mathbf{M} = (M_x, M_y, M_z)$ as a function of time when relaxation times T_1 and T_2 are present. Recently, some fractional models have been proposed for the Bloch equations, however, effective numerical methods and supporting error analyses for the fractional Bloch equation (FBE) are still limited.

In this paper, the time-fractional Bloch equations (TFBE) and the anomalous fractional Bloch equations (AFBE) are considered. Firstly, we derive an analytical solution for the TFBE with an initial condition. Secondly, we propose an effective predictor-corrector method (PCM) for the TFBE, and the error analysis for PCM is investigated. Furthermore, we derive an effective implicit numerical method (INM) for the anomalous fractional Bloch equations (AFBE), and the stability and convergence of the INM are investigated. We prove that the implicit numerical method for the AFBE is unconditionally stable and convergent. Finally, we present some numerical results that support our theoretical analysis.

Key words: Time fractional Bloch equations, anomalous fractional Bloch equations, implicit numerical method, predictor-corrector method, stability, convergence

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1. Introduction

Diffusion-weighted imaging is an MR imaging modality that allows the magnitude of the local diffusion of spins in a chosen direction to be estimated in individual scan voxels. By combining measurements in six or more directions it is possible to construct the diffusion tensor [1], which contains information describing the anisotropy of diffusion assuming Gaussian diffusion.

In physics and chemistry, specifically in NMR (nuclear magnetic resonance) or MRI (magnetic resonance imaging), or ESR (electron spin resonance) the Bloch equations are a set of macroscopic equations that are used to calculate the nuclear magnetization $\mathbf{M} = (M_x, M_y, M_z)$ as a function of time when relaxation times T_1 and T_2 are present. Here $M_x(t), M_y(t)$ and $M_z(t)$ represent the system magnetization (x, y, and z components), T_1 is the spin-lattice relaxation time characterizing the rate at which the longitudinal M_z component of the magnetization vector recovers exponentially towards its thermodynamic equilibrium, and T_2 is the spin-spin relaxation time characterizing the signal decay in NMR and MRI.

The classical Bloch equations take the following form [2, 3]:

$$\frac{dM_x(t)}{dt} = \omega_0 M_y(t) - \frac{M_x(t)}{T_2}, \tag{1}$$

$$\frac{dM_y(t)}{dt} = -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \tag{2}$$

$$\frac{dM_z(t)}{dt} = \frac{M_0 - M_z(t)}{T_1}, \tag{3}$$

where M_0 is the equilibrium magnetization, and ω_0 is the resonant frequency given by the Larmor relationship $\omega_0 = \gamma B_0$, where B_0 is the static magnetic field (z-component) and $\gamma/2\pi$ is the gyromagnetic ratio (42.57 MHz/Tesla for water protons).

Some fractional models have been proposed for the Bloch equation. Magin et al. [2] considered the following time-fractional Bloch equations (TFBE):

$${}_0^C D_t^{\alpha} M_x(t) = \omega_0' M_y(t) - \frac{M_x(t)}{T_2'}, \tag{4}$$

$${}_0^C D_t^{\alpha} M_y(t) = -\omega_0' M_x(t) - \frac{M_y(t)}{T_2'}, \tag{5}$$

$${}_0^C D_t^{\alpha} M_z(t) = \frac{M_0 - M_z(t)}{T_1'}, \tag{6}$$

where ${}_0^C D_t^{\alpha}$ is the Caputo time fractional derivative of order α ($0 < \alpha \leq 1$), and $\omega_0' = \omega_0/\tau_2^{\alpha-1}$, $1/T_1' = \tau_1^{\alpha-1}/T_1$ and $1/T_2' = \tau_2^{\alpha-1}/T_2$ each have the units of $(sec)^{-\alpha}$. The fractional time constants τ_1 and τ_2 are needed to maintain a consistent set of units for the magnetization. They used this model to study the spin dynamics and magnetization relaxation, in the simple case of a single spin particle at resonance in a static magnetic field.

Velasco et al. [3] investigated the following anomalous fractional Bloch equations (AFBE):

$$\frac{dM_x(t)}{dt} = \omega_0 M_y(t) - \frac{D_{0+}^{1-\alpha} M_x(t)}{T_2}, \tag{7}$$

$$\frac{dM_y(t)}{dt} = -\omega_0 M_x(t) - \frac{D_{0+}^{1-\alpha} M_y(t)}{T_2}, \tag{8}$$

$$\frac{dM_z(t)}{dt} = D_{0+}^{1-\beta} \frac{M_0 - M_z(t)}{T_1}, \tag{9}$$

where $D_{0+}^{1-\alpha}$ and $D_{0+}^{1-\beta}$ are the time fractional Riemann-Liouville derivative with $0 < \alpha \leq 1$ and $0 < \beta \leq 1$. They used this model to fit the derived spin-spin relaxation (T_2) decay curves to relaxation data from normal and trypsin-digested bovine nasal cartilage.

Magin et al. [2] and Velasco et al. [3] have demonstrated that a fractional calculus based diffusion model can be successfully applied to analyzing diffusion images of human brain tissues and provided new insights into further investigations of tissue structures and the microenvironment. However, effective numerical methods and supporting error analyses for the fractional Bloch equation (FBE) are still limited. This motivates us to derive an analytical solution and an effective numerical method for the FBE, and to study the stability and convergence of the proposed numerical method.

For convenience, the TFBE (4)-(6) are decoupled, which is equivalent to solving

$${}_0^C D_t^{\alpha} M(t) = -K_1 M(t) + f(t), \tag{10}$$

where $K_1 > 0$ is constant, and similarly, the AFBE (7)-(10) are decoupled, which is equivalent to solving

$$\frac{dM(t)}{dt} = -K_2 D_{0+}^{1-\alpha} M(t) + f(t), \tag{11}$$

where $K_2 > 0$ is constant. As usual we demand that the function f be continuous and that it fulfils a Lipschitz condition with respect to its second argument, with Lipschitz constant L on a suitable set G.

In this paper, we consider the time-fractional Bloch equations (TFBE) and the anomalous fractional Bloch equations (AFBE) with an initial condition.

The structure of the remainder of this paper as follows. In Section 2, some mathematical preliminaries are introduced. In Section 3, an approximate analytical solution for the TFBE is derived. In Section 4, we propose an effective predictor-corrector method (PCM) for the TFBE. The error analysis for PCM is investigated in Section 5. In Section 6, we propose an implicit numerical method (INM) for the AFBE. The stability and convergence of the INM are investigated in Sections 7 and 8, respectively. Finally, we present some numerical results that support our theoretical analysis.

2. Preliminary Knowledge

In this section, we outline important definitions and lemma used throughout the remaining sections of this paper.

Firstly, we present the definitions of two classical Mittag-Leffler functions. More detailed information on the Mittag-Leffler functions may be found in [4, 5, 6].

Definition 1. *A two-parameter function of the Mittag-Leffler type is defined by the series expansion [7]*

$$E_{\alpha,\beta}(z) \equiv \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad (\alpha > 0, \beta > 0).$$

When $\beta = 1$, we obtain the Mittag-Leffler function defined in terms of one parameter:

$$E_{\alpha,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} \equiv E_{\alpha}(z).$$

Definition 2. *Let $\boldsymbol{A} \in \mathbb{R}^{n\times n}$. The matrix $\alpha-$Exponential function $e_{\alpha}^{z\boldsymbol{A}}$ is defined by [6, 8]*

$$e_{\alpha}^{z\boldsymbol{A}} \equiv z^{\alpha-1}E_{\alpha,\alpha}(z^{\alpha}\boldsymbol{A}) = z^{\alpha-1}\sum_{k=0}^{\infty} \boldsymbol{A}^k \frac{z^{\alpha k}}{\Gamma[(k+1)\alpha]},$$

where $z \in \mathbb{C} \setminus \{0\}, \alpha > 0$.

When $\alpha = 1$, $e_1^{z\mathbf{A}}$ coincides with the matrix exponential function $e^{z\mathbf{A}}$:

$$e_1^{z\mathbf{A}} = e^{z\mathbf{A}}, (z \in \mathbb{C}).$$

In addition, the function $e_\alpha^{z\mathbf{A}}$ satisfies the following properties [6, 8]:

Lemma 1. *If $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{n\times n}$, $0 < \alpha \leq 1$, and let $\|\boldsymbol{A}\| = \max_{1\leq i,j\leq n} |a_{ij}|$, we have*

$$\begin{array}{ll} 1. & \|e_\alpha^{z\boldsymbol{A}}\| \leq |z|^{\alpha-1} \sum\limits_{k=0}^{\infty} \|\boldsymbol{A}\|^k \frac{|z|^{\alpha k}}{\Gamma[(k+1)\alpha]}, \\ 2. & e_\alpha^{z\boldsymbol{A}} e_\alpha^{z\boldsymbol{B}} \neq e_\alpha^{z(\boldsymbol{A}+\boldsymbol{B})}, (\alpha \neq 1), \\ 3. & {}_a^C D_t^\alpha e_\alpha^{z\boldsymbol{A}} = \boldsymbol{A} e_\alpha^{z\boldsymbol{A}}. \end{array}$$

Furthermore, we give the definitions of two fractional derivatives.

Definition 3. *For functions $M(t)$ given in the interval $[a, b]$, the expression [5, 9]*

$${}_a^C D_t^\alpha M(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \int_a^t \frac{M^{(m)}(\eta)}{(t-\eta)^{1+\alpha-m}} d\eta, & m-1 < \alpha < m, \\ \frac{d^m}{dt^m} M(t), & \alpha = m \in \mathbb{N}, \end{cases}$$

is called a time Caputo fractional derivative of order α $(m - 1 < \alpha \leq m)$.

Definition 4. *For functions $M(t)$ given in the interval $[a, b]$, the expression [5, 10]*

$$D_{a+}^\alpha M(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial t^m} \int_a^t \frac{M(\xi) d\xi}{(t-\xi)^{\alpha+1-m}}, & m-1 < \alpha < m, \\ \frac{d^m}{dt^m} M(t), & \alpha = m \in \mathbb{N}, \end{cases}$$

is called the Riemann-Liouville derivative of order α $(m - 1 < \alpha \leq m)$.

The relationship between the Riemann-Liouville and Caputo fractional derivative is given in [5] as

$$D_{a+}^\alpha M(t) = \sum_{j=0}^{m-1} \frac{M^j(a)}{\Gamma(1+j-\alpha)} (t-a)^{j-\alpha} + {}_a^C D_t^\alpha M(t).$$

Lemma 2. *[11, 12] Let $M \in C^m[0, T]$ for some $m \in \mathbb{N}$ and assume that $0 < \alpha < m$. Then ${}_0^C D_t^\alpha M \in C[0, T]$.*

The following properties of the operators ${}_a^C D_t^\alpha$ and D_{a+}^α are detailed in [5]:

Lemma 3. *If $\alpha \geq 0$ and $\gamma > -1$, we have*

$$\begin{array}{rcl} 1.\ {}_a^C D_t^\alpha t^\gamma & = & \frac{\Gamma(\gamma+1)}{\Gamma(\gamma-\alpha+1)}(t-a)^{\gamma-\alpha}, \\ 2.\ D_{a+}^\alpha t^\gamma & = & \frac{\Gamma(\gamma+1)}{\Gamma(\gamma-\alpha+1)}(t-a)^{\gamma-\alpha}. \end{array}$$

Noting that for constant C^*, ${}_a^C D_t^\alpha C^* = 0$ and $D_{a+}^\alpha C^* = \frac{C^*(t-a)^{-\alpha}}{\Gamma(1-\alpha)}$.

3. Analytical solution of the TFBE

The time-fractional Bloch equations (TFBE) (4)-(6) can be written as

$$ {}_0^C D_t^\alpha \bar{M}(t) = \mathbf{A}\bar{M}(t) + \bar{b}(t), \tag{12}$$

which satisfies

$$\bar{M}(0) = \bar{M}_0, \tag{13}$$

where $\mathbf{A} = \begin{pmatrix} -\frac{1}{T_2'} & \omega_0' & 0 \\ -\omega_0' & -\frac{1}{T_2'} & 0 \\ 0 & 0 & -\frac{1}{T_1'} \end{pmatrix}$ is a 3×3 constant matrix, $\bar{b}(t) = (0, 0, \frac{M_0}{T_1'})^T$, $\bar{M}(t) = (M_x(t), M_y(t), M_z(t))^T$ and $\bar{M}_0 = (M_x(0), M_y(0), M_z(0))^T$ are vectors.

Lemma 4. *The matrix*

$$\boldsymbol{T}(t) = e_\alpha^{t\boldsymbol{A}}, \quad \left(\boldsymbol{A} \in \mathbb{R}^{n\times n}\right)$$

is a fundamental solution matrix for the system

$${}_0^C D_t^\alpha \bar{M}(t) = \boldsymbol{A}\bar{M}(t).$$

Theorem 1. *The following initial-value problem*

$$\begin{array}{rcl} {}_0^C D_t^\alpha \bar{M}(t) & = & \boldsymbol{A}\bar{M}(t), \\ \bar{M}(0) & = & \bar{M}_0 \quad (\bar{M}_0 \in \mathbb{R}^n), \end{array}$$

where $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, has its unique continuous global solution $\bar{M}(t)$ in $[0,\infty) \subset \mathbb{R}$ given by

$$\bar{M}(t) = \int_0^t e_\alpha^{(t-\xi)\boldsymbol{A}} \boldsymbol{A}\bar{M}_0 d\xi + \bar{M}_0.$$

PROOF. See [6, 8].

Using $\mathbb{C}_\gamma[a,b]$ $(\gamma \in \mathbb{R})$ [6, 8] to denote the Banach space

$$\mathbb{C}_\gamma[a,b] = \{f(t) \in C(a,b] : \|f\|_{\mathbb{C}_\gamma} = \|(t-a)^\gamma f(t)\|_C < \infty\},$$

where $\|f\|_C = \max_{t\in[a,b]} |f(t)|$. In particular, $\mathbb{C}_0[a,b]$ represents the space of continuous functions in $[a,b]$, namely $C[a,b]$.

Then, using Lemma 1, Lemma 2, Lemma 4 and Theorem 1, we can obtain an explicit general solution of the time-fractional Bloch equations (TFBE) (12)-(13) by Theorem 2.

Theorem 2. *The following initial-value problem*

$$\begin{aligned} {}_0^C D_t^\alpha \bar{M}(t) &= \boldsymbol{A}\bar{M}(t) + \bar{b}(t), \\ \bar{M}(0) &= \bar{M}_0 \quad (\bar{M}_0 \in \mathbb{R}^n), \end{aligned}$$

where $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ *and* $\bar{b} \in \bar{\mathbb{C}}_{1-\alpha}[0,T]$*, meaning each component of* $\bar{b}$ *belongs to space* $\mathbb{C}_{1-\alpha}[0,T]$*, has its unique solution given by*

$$\begin{aligned} \bar{M}(t) &= \int_0^t e_\alpha^{(t-\xi)\boldsymbol{A}}[\bar{b}(\xi) + \boldsymbol{A}\bar{M}_0]d\xi + \bar{M}_0 \\ &= \int_0^t e_\alpha^{(t-\xi)\boldsymbol{A}}\bar{b}(\xi)d\xi + [\boldsymbol{A}t^\alpha E_{\alpha,\alpha+1}(t^\alpha \boldsymbol{A}) + I]\,\bar{M}_0. \end{aligned}$$

PROOF. See [6, 8].

4. An effective predictor-corrector method (PCM) for the TFBE

We propose an effective predictor-corrector method (PCM) for the following time-fractional Bloch equation (TFBE) with initial condition:

$$\begin{aligned} {}_0^C D_t^\alpha M(t) &= -K_1 M(t) + f(t), && (14) \\ M(0) &= M_0^\#, && (15) \end{aligned}$$

where $0 < \alpha \leq 1$, and $K_1 > 0$, $M_0^\#$ are constants.

It is well known that the initial value problem (14)-(15) is equivalent to the Volterra integral equation

$$M(t) = M_0^\# + \frac{1}{\Gamma(\alpha)}\int_0^t (t-\xi)^{\alpha-1}[-K_1 M(\xi) + f(\xi)]d\xi.$$

For the sake of simplicity, we assume that we are working with a uniform temporal discrete scheme $t_j = j\tau, j = 0, 1, \cdots, n$, and $n\tau = T$, where T represents the final time.

It is known that the classical Adams-Bashforth-Moulton method for first order ordinary differential equations is a reasonable and practically useful compromise in the sense that its stability properties allow for a safe application to mildly stiff equations without undue propagation of rounding error, whereas the implementation does not require extremely time consuming elements [13]. Thus, a fractional Adams-Bashforth method and a fractional Adams-Moulton method are chosen as our predictor and corrector formulas.

The predictor M^p_{k+1} is determined by the fractional Adams-Bashforth method [11, 12, 14]:

$$M^p_{k+1} = M^{\#}_0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{k} b_{j,k+1}[-K_1 M_j + f(t_j)], \tag{16}$$

where

$$b_{j,k+1} = \frac{\tau^\alpha}{\alpha}[(k+1-j)^\alpha - (k-j)^\alpha]. \tag{17}$$

Remark 1. *[14] $b_{j,k+1} > 0$ for all j and k, and*

$$\sum_{j=0}^{k} b_{j,k+1} = \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} dt = \frac{1}{\alpha} t^\alpha_{k+1} \le \frac{1}{\alpha} T^\alpha.$$

The fractional Adams-Moulton method determines the corrector formula [11, 12, 14]:

$$\begin{aligned} M_{k+1} \quad &= M^{\#}_0 + \frac{1}{\Gamma(\alpha)}(\sum_{j=0}^{k} a_{j,k+1}[-K_1 M_j + f(t_j)] \\ &+ a_{k+1,k+1}[-K_1 M^p_{k+1} + f(t_{k+1})]), \end{aligned} \tag{18}$$

where

$$a_{j,k+1} = \frac{\tau^\alpha}{\alpha(\alpha+1)} \begin{cases} k^{\alpha+1} - (k-\alpha)(k+1)^\alpha, & j = 0, \\ (k-j+2)^{\alpha+1} + (k-j)^{\alpha+1} & \\ \quad -2(k-j+1)^{\alpha+1}, & 1 \le j \le k, \\ 1, & j = k+1. \end{cases} \tag{19}$$

Remark 2. *[14]* $a_{j,k+1} > 0$ *for all* j *and* k*, and*

$$\sum_{j=0}^{k} a_{j,k+1} = \int_0^{t_k} (t_k - t)^{\alpha-1} dt = \frac{1}{\alpha} t_k^\alpha \leq \frac{1}{\alpha} T^\alpha.$$

This method has been used for parameter estimation of fractional dynamical models arising from biological systems [15].

5. Error analysis for predictor-corrector method (PCM)

In this section, we present the theorems concerning the error of our fractional predictor-corrector method (PCM).

Lemma 5. *Let* $z \in C^1[0, T]$*, then*

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} z(t) dt - \sum_{j=0}^{k} b_{j,k+1} z(t_j) \right| \leq \frac{1}{\alpha} \|z'\|_\infty t_{k+1}^\alpha \tau,$$

where $\|z\|_\infty = \max\limits_{0 \leq t \leq T} |z(t)|$.

Proof. See [12].

Lemma 6. *If* $z \in C^2[0, T]$*, then there is a constant* C_α *depending only on* α *such that*

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} z(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} z(t_j) \right| \leq C_\alpha \|z''\|_\infty t_{k+1}^\alpha \tau^2.$$

Proof. See [12].

Theorem 3. *If* ${}_0^C D_t^\alpha M \in C^2[0, T]$*, then*

$$\max_{0 \leq j \leq n} |M(t_j) - M_j| = O(\tau^{1+\alpha}).$$

PROOF. Using the given condition ${}_0^C D_t^\alpha M \in C^2[0,T]$, together with Lemmas 5 and 6, we have

$$\left| \int_0^{t_{k+1}} (t_{k+1}-t)^{\alpha-1} \, {}_0^C D_t^\alpha M(t) dt - \sum_{j=0}^{k} b_{j,k+1} \, {}_0^C D_t^\alpha M(t_j) \right| \le C_1 t_{k+1}^\alpha \tau, \quad (20)$$

and

$$\left| \int_0^{t_{k+1}} (t_{k+1}-t)^{\alpha-1} \, {}_0^C D_t^\alpha M(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} \, {}_0^C D_t^\alpha M(t_j) \right| \le C_2 t_{k+1}^\alpha \tau^2. \quad (21)$$

We will show that, for sufficiently small $\tau = T/n$,

$$\max_{0 \le j \le n} |M(t_j) - M_j| = O(\tau^{1+\alpha}). \quad (22)$$

The proof will be based on mathematical induction. In view of the given initial condition, the induction basis ($j = 0$) is presupposed.

Now assume that (22) is true for $j = 0, 1, \cdots, k (k \le n-1)$, that is

$$\max_{0 \le j \le k} |M(t_j) - M_j| = O(\tau^{1+\alpha}). \quad (23)$$

We must then prove that the inequality also holds for $j = k+1$. To do this, we first look at the error of the predictor M_{k+1}^p. By construction of the predictor, using (20), assumption (23), Remark 1, and $-K_1 M(t) + f(t)$ fulfils a Lipschitz condition, we find that

$$\begin{aligned}
&|M(t_{k+1}) - M_{k+1}^p| \\
&= \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_{k+1}} (t_{k+1}-t)^{\alpha-1} [-K_1 M(t) + f(t)] dt \right. \\
&\left. - \sum_{j=0}^{k} b_{j,k+1} [-K_1 M_j + f(t_j)] \right| \\
&\le \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_{k+1}} (t_{k+1}-t)^{\alpha-1} \, {}_0^C D_t^\alpha M(t) dt - \sum_{j=0}^{k} b_{j,k+1} \, {}_0^C D_t^\alpha M(t_j) \right|
\end{aligned}$$

$$+\frac{1}{\Gamma(\alpha)}\sum_{j=0}^{k} b_{j,k+1}|[-K_1M(t_j)+f(t_j)]-[-K_1M_j+f(t_j)]|$$
$$\leq \frac{C_1t_{k+1}^{\alpha}}{\Gamma(\alpha)}\tau+\frac{1}{\Gamma(\alpha)}\sum_{j=0}^{k} b_{j,k+1}LC\tau^{1+\alpha}$$
$$\leq \frac{C_1T^{\alpha}}{\Gamma(\alpha)}\tau+\frac{CLT^{\alpha}}{\Gamma(\alpha+1)}\tau^{1+\alpha}. \tag{24}$$

On the basis of the bound (24) for the predictor error, we begin the analysis of the corrector error. We recall the relation (19) which we shall use, in particular, for $j=k+1$ and arguing in a similar way to the above, using (21), (24), assumption (23), Remark 2, and $-K_1M(t)+f(t)$ fulfils a Lipschitz condition, we find that

$$|M(t_{k+1})-M_{k+1}|$$
$$=\frac{1}{\Gamma(\alpha)}\left|\int_0^{t_{k+1}}(t_{k+1}-t)^{\alpha-1}[-K_1M(t)+f(t)]dt\right.$$
$$\left.-\sum_{j=0}^{k} a_{j,k+1}[-K_1M_j+f(t_j)]-a_{k+1,k+1}[-K_1M_{k+1}^p+f(t_{k+1})]\right|$$
$$\leq \frac{1}{\Gamma(\alpha)}\left|\int_0^{t_{k+1}}(t_{k+1}-t)^{\alpha-1}\,{}_0^CD_t^{\alpha}M(t)dt-\sum_{j=0}^{k+1} a_{j,k+1}\,{}_0^CD_t^{\alpha}M(t_j)\right|$$
$$+\frac{1}{\Gamma(\alpha)}\sum_{j=0}^{k} a_{j,k+1}|[-K_1M(t_j)+f(t_j)]-[-K_1M_j+f(t_j)]|$$
$$+\frac{1}{\Gamma(\alpha)}a_{k+1,k+1}|[-K_1M(t_{k+1})+f(t_{k+1})]-[-K_1M_{k+1}^p+f(t_{k+1})]|$$
$$\leq \frac{C_2t_{k+1}^{\alpha}}{\Gamma(\alpha)}\tau^2+\frac{CL}{\Gamma(\alpha)}\tau^{1+\alpha}\sum_{j=0}^{k} a_{j,k+1}$$
$$+a_{k+1,k+1}\frac{L}{\Gamma(\alpha)}\left(\frac{C_1T^{\alpha}}{\Gamma(\alpha)}\tau+\frac{CLT^{\alpha}}{\Gamma(\alpha+1)}\tau^{1+\alpha}\right)$$

$$\leq \left(\frac{C_2 T^\alpha}{\Gamma(\alpha)} + \frac{CLT^\alpha}{\Gamma(\alpha+1)} + \frac{C_1 LT^\alpha}{\Gamma(\alpha)\Gamma(\alpha+2)} + \frac{CL^2 T^\alpha}{\Gamma(\alpha+1)\Gamma(\alpha+2)} \tau^\alpha \right) \tau^{1+\alpha}$$
$$\leq C_0 \tau^{1+\alpha}.$$

Thus, we now see that the induction step is completed and the result is true for all j.

6. Implicit numerical method for the AFBE

In this section, we propose an implicit numerical method (INM) for the following anomalous fractional Bloch equations (AFBE) with initial condition:

$$\frac{dM(t)}{dt} = -K_2 D_{0+}^{1-\alpha} M(t) + f(t), 0 \leq t \leq T, \tag{25}$$
$$M(0) = M_0^*, \tag{26}$$

where $K_2 > 0$ and M_0^* are constants, and $D_{0+}^{1-\alpha}(0 < \alpha \leq 1)$ is the time fractional Riemann-Liouville derivative and can be written as [5]

$$D_{0+}^{1-\alpha} M(t) = \frac{\partial}{\partial t} I_0^\alpha M(t),$$

where $I_0^\alpha M(t) = \frac{1}{\Gamma(\alpha)} \int_0^t \frac{M(\eta)d\eta}{(t-\eta)^{1-\alpha}}$ is the Riemann-Liouville fractional integral of order $\alpha > 0$.

Let $t = t_k = k\tau (k = 0, 1, \cdots, n)$, where $\tau = T/n$ is the time step size.

We introduce the following numerical approximation

$$\begin{aligned} I_0^\alpha M(t_k) &= \frac{1}{\Gamma(\alpha)} \int_0^{t_k} \frac{M(\eta)}{(t_k-\eta)^{1-\alpha}} d\eta \\ &= \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{M(\eta)}{(t_k-\eta)^{1-\alpha}} d\eta \\ &= \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{M(t_{j+1}) + M'(\eta_j)(\eta - t_{j+1})}{(t_k-\eta)^{1-\alpha}} d\eta \\ &= \frac{\tau^\alpha}{\Gamma(\alpha+1)} \sum_{j=0}^{k-1} b_j M(t_{k-j}) + Ck^\alpha \tau^{1+\alpha} \max_{0\leq t\leq T} |M'(t)|, \end{aligned}$$

where $t_j < \eta_j < t_{j+1}$, and $b_j = (j+1)^\alpha - j^\alpha, j = 0, 1, \cdots, n-1$.

Thus, we have

Lemma 7. *If $M(t) \in C^1[0,T]$, then*

$$I_0^\alpha M(t_k) = \frac{\tau^\alpha}{\Gamma(\alpha+1)} \sum_{j=0}^{k-1} b_j M(t_{k-j}) + R_k^\alpha,$$

where $|R_k^\alpha| \leq C t_k^\alpha \tau$.

Lemma 8. *The coefficients b_j satisfy*

(1) *$b_j > 0$ for $j = 0, 1, 2, \cdots$;*
(2) *$1 = b_0 > b_1 > \cdots > b_n$, $b_n \to 0$ as $n \to \infty$;*
(3) *There exists a positive constant $C > 0$, such that $\tau \leq C b_j \tau^\alpha, j = 1, 2, \cdots$;*
(4) *$\sum_{j=0}^{k} b_j \tau^\alpha = (k+1)^\alpha \tau^\alpha \leq T^\alpha$.*

Proof. See [16].

Using Lemmas 7 and 8, we have the following Lemma.

Lemma 9. *If $M(t) \in C^2[0,T]$, then*

$$\begin{aligned} &I_0^\alpha M(t_{k+1}) - I_0^\alpha M(t_k) \\ &= \frac{\tau^\alpha}{\Gamma(\alpha+1)} \left\{ b_k M(t_1) + \sum_{j=0}^{k-1} b_{k-j-1}[M(t_{j+2}) - M(t_{j+1})] \right\} + R_{k,\alpha}, \end{aligned}$$

where $|R_{k,\alpha}| \leq C b_k \tau^{1+\alpha}$.

Proof. See [17].

Integrating both sides of Eq.(25) from t_k to t_{k+1}, we have

$$M(t_{k+1}) - M(t_k) = -K_2[I_0^\alpha M(t_{k+1}) - I_0^\alpha M(t_k)] + \int_{t_k}^{t_{k+1}} f(t)dt.$$

Thus, using Lemma 9 we have

$$
\begin{aligned}
M(t_{k+1}) &= M(t_k) - r\left\{ b_k M(t_1) - \sum_{j=0}^{k-1} b_{k-j-1}[M(t_{j+2}) - M(t_{j+1})] \right\} \\
&+ \frac{\tau}{2}[f(t_{k+1}) + f(t_k)] + R_{k+1},
\end{aligned}
$$

or, rearranging, we obtain

$$
\begin{aligned}
M(t_{k+1}) &= M(t_k) - rM(t_{k+1}) - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)M(t_{k-j}) \\
&+ \frac{\tau}{2}[f(t_{k+1}) + f(t_k)] + R_{k+1}, \\
& k = 0, 1, 2, \cdots, n-1,
\end{aligned} \tag{27}
$$

where $r = \frac{K_2\tau^\alpha}{\Gamma(\alpha+1)}$, and

$$
|R_{k+1}| \leq C b_k \tau^{1+\alpha}. \tag{28}
$$

Thus, we have derived the following implicit numerical method (INM) for the initial value problem of the anomalous fractional Bloch equations (AFBE):

$$
\begin{aligned}
M^{k+1} &= M^k - rM^{k+1} - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)M^{k-j} \\
&+ \frac{\tau}{2}[f(t_{k+1}) + f(t_k)], \\
& k = 0, 1, 2, \cdots, n-1.
\end{aligned} \tag{29}
$$

7. Stability of the implicit numerical method for the AFBE

In this section, we discuss the stability of the implicit numerical method for the AFBE.

Theorem 4. *The implicit numerical method defined by Eq.(29) is unconditionally stable.*

Proof. We suppose that $\widetilde{M}^k (k = 0, 1, 2, \cdots, n)$ is the approximate solution of Eq.(29). The rounding error $\varepsilon^k = \widetilde{M}^k - M^k$ satisfies

$$
\varepsilon^{k+1} = \varepsilon^k - r\varepsilon^{k+1} - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)\varepsilon^{k-j}. \tag{30}
$$

Multiplying Eq. (30) by ε^{k+1} we obtain

$$(\varepsilon^{k+1})^2 = \varepsilon^{k+1}\varepsilon^k - r(\varepsilon^{k+1})^2 - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)\varepsilon^{k-j}\varepsilon^{k+1}.$$

Using the inequality $\pm\varepsilon^{k-j}\varepsilon^{k+1} \leq \frac{1}{2}\left[(\varepsilon^{k-j})^2 + (\varepsilon^{k+1})^2\right]$, we have

$$\begin{aligned}
(\varepsilon^{k+1})^2 &\leq \frac{1}{2}\left[(\varepsilon^{k+1})^2 + (\varepsilon^k)^2\right] - r(\varepsilon^{k+1})^2 \\
&+ \frac{r}{2}\sum_{j=0}^{k-1}(b_j - b_{j+1})\left[(\varepsilon^{k-j})^2 + (\varepsilon^{k+1})^2\right].
\end{aligned}$$

Using Lemma 8 and noting $b_0 = 1$, we have

$$\sum_{j=0}^{k-1}(b_j - b_{j+1}) = 1 - b_k,$$

and

$$\begin{aligned}
(\varepsilon^{k+1})^2 &\leq \frac{1}{2}\left[(\varepsilon^{k+1})^2 + (\varepsilon^k)^2\right] - \frac{r}{2}(1 + b_k)(\varepsilon^{k+1})^2 + \frac{r}{2}\sum_{j=0}^{k-1}(b_j - b_{j+1})(\varepsilon^{k-j})^2 \\
&\leq \frac{1}{2}\left[(\varepsilon^{k+1})^2 + (\varepsilon^k)^2\right] - \frac{r}{2}(\varepsilon^{k+1})^2 + \frac{r}{2}\sum_{j=0}^{k-1}(b_j - b_{j+1})(\varepsilon^{k-j})^2.
\end{aligned}$$

Therefore, we obtain

$$(\varepsilon^{k+1})^2 + r\sum_{j=0}^{k} b_j(\varepsilon^{k+1-j})^2 \leq (\varepsilon^k)^2 + r\sum_{j=0}^{k-1} b_j(\varepsilon^{k-j})^2.$$

Let

$$(\varepsilon^k)_E^2 = (\varepsilon^k)^2 + r\sum_{j=0}^{k-1} b_j(\varepsilon^{k-j})^2,$$

we obtain the result

$$(\varepsilon^{k+1})^2 \leq (\varepsilon^{k+1})_E^2 \leq (\varepsilon^k)_E^2 \leq \cdots \leq (\varepsilon^1)_E^2 \leq (\varepsilon^0)_E^2 = (\varepsilon^0)^2.$$

Hence, the proof of Theorem 4 is completed.

8. Convergence of the implicit numerical method for the AFBE

Let $M(t_k)(k = 0, 1, 2, \cdots, n)$ be the exact solution of the anomalous fractional Bloch equations (AFBE) (25)-(26) at mesh point t_k. Define $\eta^k = M(t_k) - M^k(k = 0, 1, 2, \cdots, n)$.

We will prove the following theorem of convergence.

Theorem 5. *The implicit numerical method defined by Eq.(25) is convergent, and there exists a positive constant $C^* > 0$, such that*

$$|\eta^{k+1}| \leq C^* \tau, k = 0, 1, 2, \cdots, n-1.$$

Proof. From Eq. (27) and Eq. (29), we have

$$\begin{aligned} \eta^{k+1} &= \eta^k - r\eta^{k+1} - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)\eta^{k-j} + R_{k+1}, \\ & k = 0, 1, 2, \cdots, n-1. \end{aligned} \tag{31}$$

Multiplying Eq. (31) by η^{k+1} and using the Cauchy-Schwartz inequality we obtain

$$\begin{aligned} (\eta^{k+1})^2 &= \eta^{k+1}\eta^k - r(\eta^{k+1})^2 - r\sum_{j=0}^{k-1}(b_{j+1} - b_j)\eta^{k-j}\eta^{k+1} + R_{k+1}\eta^{k+1} \\ &\leq \frac{1}{2}\left[(\eta^{k+1})^2 + (\eta^k)^2\right] - \frac{r}{2}(1 + b_k)(\eta^{k+1})^2 \\ &\quad + \frac{r}{2}\sum_{j=0}^{k-1}(b_j - b_{j+1})(\eta^{k-j})^2 + R_{k+1}\eta^{k+1}. \end{aligned}$$

Let

$$(\eta^k)_E^2 = (\eta^k)^2 + r\sum_{j=0}^{k-1} b_j(\eta^{k-j})^2,$$

Using the result $uv \leq \sigma u^2 + \frac{1}{4\sigma}v^2, \sigma > 0$, we have

$$R_{k+1}\eta^{k+1} \leq \frac{rb_k}{2}(\eta^{k+1})^2 + \frac{1}{2rb_k}(R_{k+1})^2.$$

Therefore, using Lemma 8, we obtain

$$\begin{aligned}
(\eta^{k+1})_E^2 &= (\eta^{k+1})^2 + r\sum_{j=0}^{k} b_j(\eta^{k+1-j})^2 \\
&\le (\eta^k)^2 + r\sum_{j=0}^{k-1} b_j(\eta^{k-j})^2 - \frac{r}{2}b_k(\eta^{k+1})^2 + R_{k+1}\eta^{k+1} \\
&= (\eta^k)_E^2 - \frac{r}{2}b_k(\eta^{k+1})^2 + R_{k+1}\eta^{k+1} \\
&\le (\eta^k)_E^2 - \frac{r}{2}b_k(\eta^{k+1})^2 + \frac{rb_k}{2}(\eta^{k+1})^2 + \frac{1}{2rb_k}(R_{k+1})^2 \\
&\le (\eta^k)_E^2 + Cb_k\tau^{2+\alpha} \\
&\le (\eta^0)_E^2 + C\sum_{j=0}^{k} b_k\tau^\alpha\tau^2 \\
&\le (C^*\tau)^2,
\end{aligned}$$

i.e. $|\eta^{k+1}| \le |\eta^{k+1}|_E \le C^*\tau$. Hence, the proof of Theorem 5 is completed.

9. Numerical results

In this section, we present some numerical examples that support our theoretical analysis.

Example 1. In order to show the efficiency of the predictor-corrector method (PCM), we consider the following time-fractional Bloch equation (TFBE) with initial condition:

$$\begin{aligned}
{}_0^C D_t^\alpha M(t) &= -K_1 M(t) + f(t), 0 \le t \le T, \\
M(0) &= 0,
\end{aligned}$$

where $0 < \alpha \le 1, K_1 > 0$, and $f(t) = K_1 t^\alpha + \Gamma(1+\alpha)$.

The exact solution of this problem is $M(t) = t^\alpha$, which can be verified by direct fractional differentiation of the given solution using Lemma 3, and substituting in the fractional differential equation. The initial condition is clearly satisfied.

When $\alpha = 0.7, K_1 = 1$, Figure 1 shows the numerical solution obtained by applying the predictor-corrector method (PCM) (16)-(19) and the exact

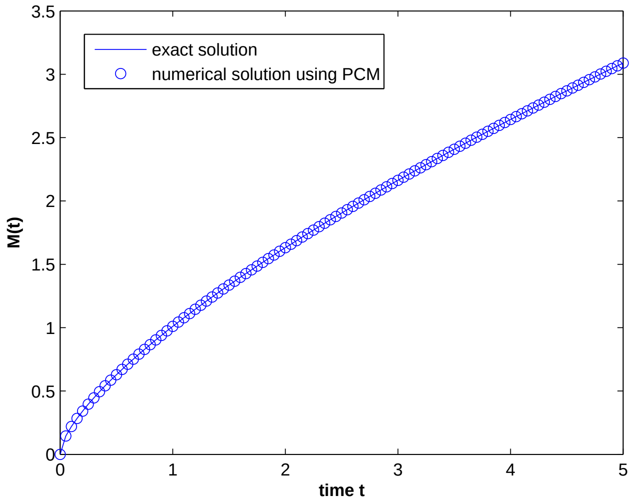


Figure 1: Comparison of the exact solution of TFBE and the numerical solution using PCM for $\alpha = 0.7, K_1 = 1$.

solution of TFBE. It can be seen that the numerical solution is in excellent agreement with the exact solution.

Example 2. Consider the following time-fractional Bloch equations (TFBE) [2] :

$$\begin{aligned} {}_0^C D_t^{\alpha} M_x(t) &= \omega_0' M_y(t) - \frac{M_x(t)}{T_2'}, \\ {}_0^C D_t^{\alpha} M_y(t) &= -\omega_0' M_x(t) - \frac{M_y(t)}{T_2'}, \\ {}_0^C D_t^{\alpha} M_z(t) &= \frac{M_0 - M_z(t)}{T_1'}, \end{aligned}$$

with initial condition

$$\begin{aligned} M_x(0) &= 0, \\ M_y(0) &= 100, \\ M_z(0) &= 0, \end{aligned}$$

where $0 < \alpha \leq 1$.

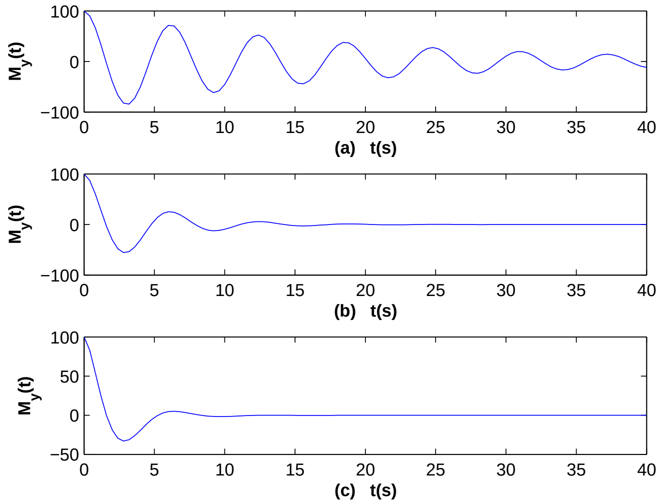
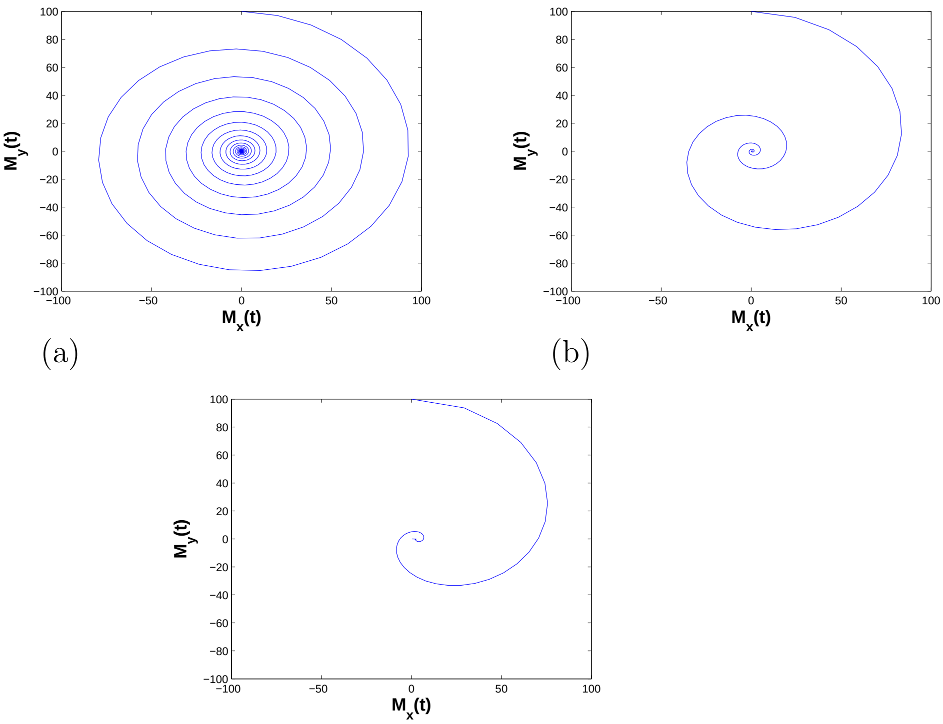


Figure 2: Plots of $M_y(t)$ of TFBE for $T_2' = 20(ms)^\alpha$ and $f_0 = (\omega_0/2\pi) = 160Hz$ and (a) $\alpha = 1.0$, (b) $\alpha = 0.9$ and (c) $\alpha = 0.8$ top to bottom, respectively.

Using the same parameters in [2], when $T_2' = 20(ms)^\alpha$ and $f_0 = (\omega_0/2\pi) = 160Hz$, Figure 2 (a)-(c) show plots of $M_y(t)$ obtained by applying the predictor-corrector method (PCM) (16)-(19) for the values of (a) $\alpha = 1.0$, (b) $\alpha = 0.9$ and (c) $\alpha = 0.8$ for a spin system.

To illustrate the dynamic relationship between the $M_x(t)$ and $M_y(t)$ for fractional and the integral order relaxation, these two components of magnetization obtained by applying the predictor-corrector method (PCM) (16)-(19) are plotted in the complex plane, as shown in Figure 3. Figure 3(a) the classical case of $\alpha = 1$ shows a regular spiral from the initial values $M_x(0) = 0$ and $M_y(0) = 100$ into the origin (center of the plot) [2]. Figure 3(b) and Figure 3(c) show a much faster decay for the chosen values of T_2' for $\alpha = 0.9$ and $\alpha = 0.8$, respectively. In Figure 4 and 5, the entire trajectory of magnetization is shown for both cases in three dimensions with the magnetization starting at $M_x(0) = 0$ and $M_y(0) = 100$ and returning to its equilibrium value of M_0.

Example 3. Consider the following anomalous fractional Bloch equa-



(a) (b) (c)

Figure 3: Plots of $M_x(t)$ and $M_y(t)$ of TFBE in the complex plane with $\alpha = 1$ (a, classical model), $\alpha = 0.9$ (b) and $\alpha = 0.8$ (c) for $T_2' = 20(ms)^\alpha$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

tions (AFBE) with initial condition:

$$\begin{aligned} \frac{dM(t)}{dt} &= -K_2 D_{0+}^{1-\alpha} M(t) + f(t), 0 \le t \le T, \\ M(0) &= 0, \end{aligned}$$

where $0 < \alpha \le 1, K_2 > 0$, and $f(t) = (1+\alpha)t^\alpha + \frac{K_2\Gamma(2+\alpha)}{\Gamma(1+2\alpha)} t^{2\alpha}$.

The exact solution of this problem is $M(t) = t^{1+\alpha}$, which can be verified by direct fractional differentiation of the given solution using Lemma 3, and substituting in the fractional differential equation. The initial condition is clearly satisfied.

When $\alpha = 0.7, K_2 = 1$, Figure 6 shows the numerical solution obtained by applying the implicit numerical method (INM) (29) and the exact solution of AFBE. It can be seen that the numerical solution is in excellent agreement with the exact solution.

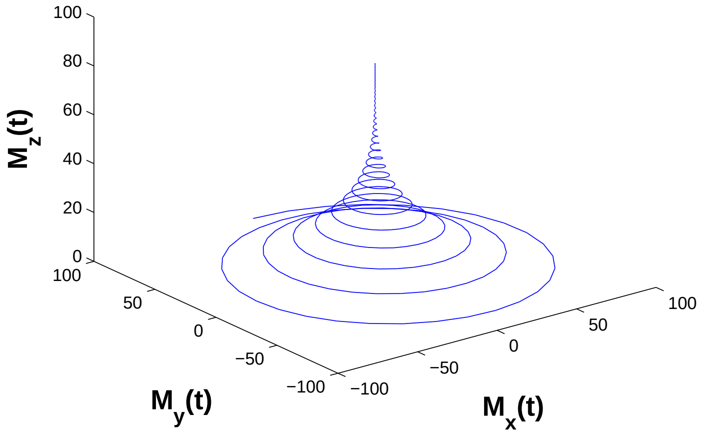


Figure 4: A Plot of numerical solutions of TFBE using the predictor-corrector method (PCM) with $\alpha = 1$ (classical model) for $T_1' = 100(ms)^\alpha$, $T_2' = 20(ms)^\alpha$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

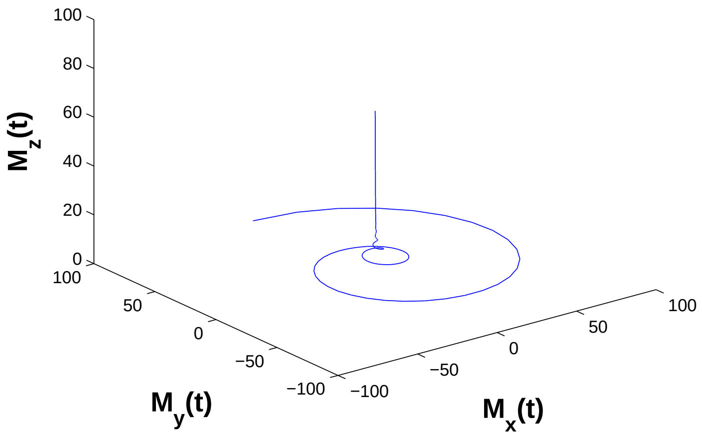


Figure 5: A Plot of numerical solutions of TFBE using the predictor-corrector method (PCM) with $\alpha = 0.9$ (fractional model) for $T_1' = 100(ms)^\alpha$, $T_2' = 20(ms)^\alpha$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

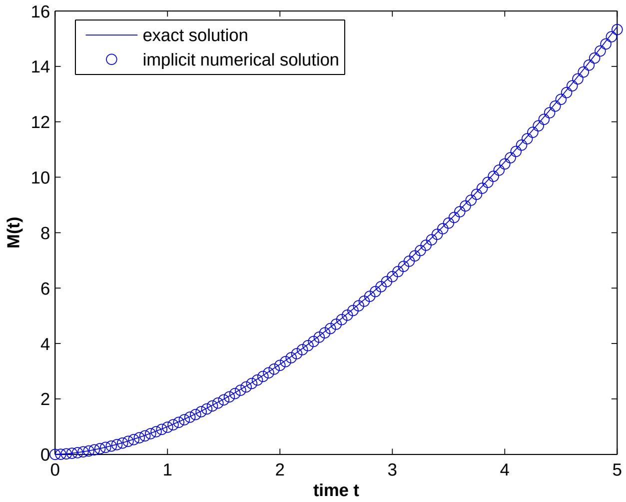


Figure 6: Comparison of the exact solution of AFBE and the numerical solution using INM for $\alpha = 0.7, K_2 = 1$.

Example 4. Consider the following anomalous fractional Bloch equations (AFBE) with initial condition:

$$\begin{aligned}
\frac{dM_x(t)}{dt} &= \omega_0 M_y(t) - \frac{D_{0+}^{1-\alpha} M_x(t)}{T_2}, \\
\frac{dM_y(t)}{dt} &= -\omega_0 M_x(t) - \frac{D_{0+}^{1-\alpha} M_y(t)}{T_2}, \\
\frac{dM_z(t)}{dt} &= D_{0+}^{1-\beta} \frac{M_0}{T_1} - D_{0+}^{1-\beta} \frac{M_z(t)}{T_1},
\end{aligned}$$

with initial condition

$$\begin{aligned}
M_x(0) &= 0, \\
M_y(0) &= 100, \\
M_z(0) &= 0,
\end{aligned}$$

where $0 < \alpha \leq 1$.

When $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$, Figure 7 (a)-(c) show plots of $M_y(t)$ obtained by applying the implicit numerical method (INM)

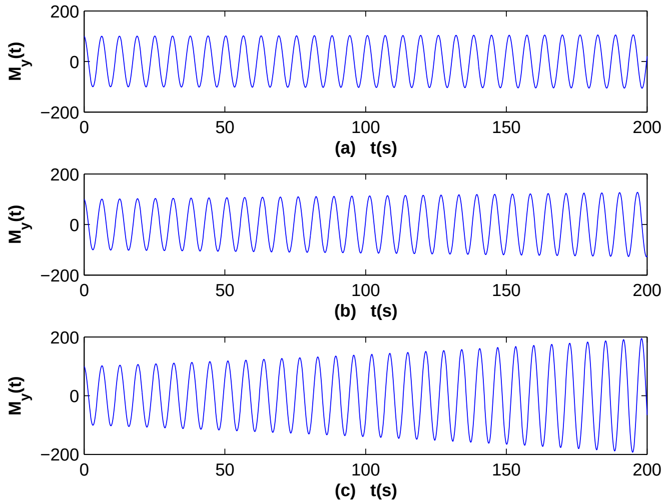


Figure 7: Plots of $M_y(t)$ of AFBE for $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$ and (a) $\alpha = 1.0$, (b) $\alpha = 0.9$ and (c) $\alpha = 0.8$ top to bottom, respectively.

(29) for the values of (a) $\alpha = 1.0$, (b) $\alpha = 0.9$ and (c) $\alpha = 0.8$ for a spin system.

Figure 8 shows the dynamic relationship between the $M_x(t)$ and $M_y(t)$ with the chosen values of T_2 for $\alpha = \beta = 1.0$, 0.9 and 0.8, respectively. Figures 9-11 exhibit the entire trajectory of magnetization in three dimensions with the magnetization starting at $M_x(0) = 0$ and $M_y(0) = 100$ and returning to its equilibrium value of M_0 for $\alpha = \beta = 1.0$, 0.9 and 0.8, respectively.

10. Conclusions

In this paper, an analytical solution and an effective predictor-corrector method (PCM) for solving the time-fractional Bloch equations (TFBE) have been derived. The error analysis for PCM is discussed. In addition, an effective implicit numerical method (INM) for solving the anomalous fractional Bloch equations (AFBE) has been proposed. The stability and convergence of the INM are analyzed systematically. We also presented some numerical examples to demonstrate the effectiveness of PCM and INM. The results show that the spin dynamics are generally fractional order, although become the classical case when the order of differentiation is one, and suggest that

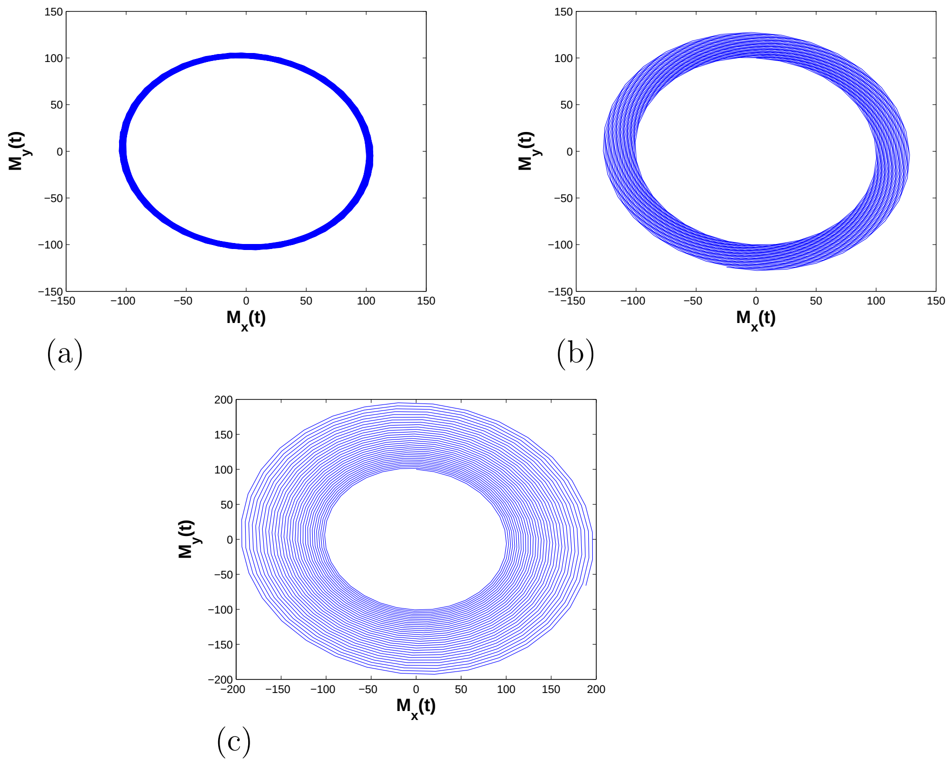


Figure 8: Plots of $M_x(t)$ and $M_y(t)$ of AFBE in the complex plane with $\alpha = 1$ (a, classical model), $\alpha = 0.9$ (b) and $\alpha = 0.8$ (c) for $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

the fractional models can effectively simulate the spin dynamics in a static magnetic field, and can play an important role for us understanding NMR for complex systems. These numerical techniques can also be applied to simulate other fractional order differential system, and therefore we feel our methods have broader application.

Acknowledgments

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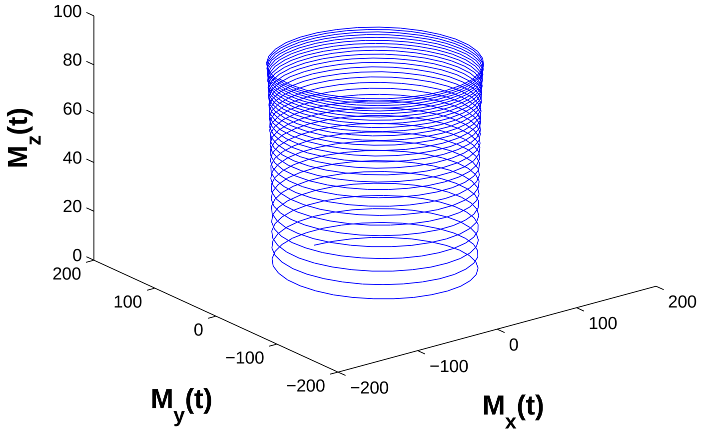

Figure 9: A Plot of numerical solutions of AFBE using the implicit numerical method (INM) with $\alpha = \beta = 1$ (classical model) for $T_1 = 100(ms)$, $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

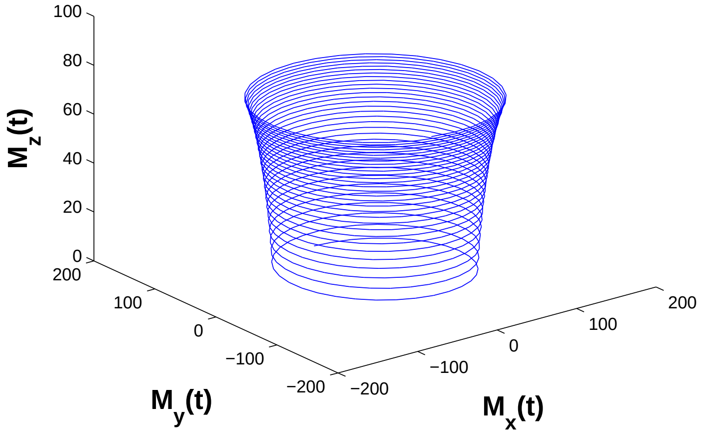

Figure 10: A Plot of numerical solutions of AFBE using the implicit numerical method (INM) with $\alpha = \beta = 0.9$ (fractional model) for $T_1 = 100(ms)$, $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

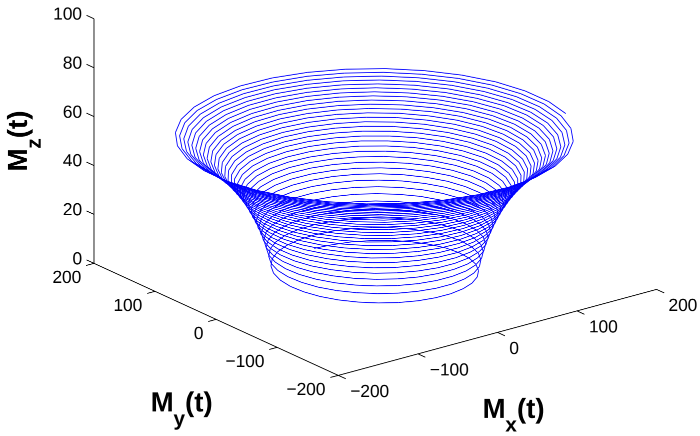

Figure 11: A Plot of numerical solutions of TFBE using the implicit numerical method (INM) with $\alpha = \beta = 0.8$ (fractional model) for $T_1 = 100(ms)$, $T_2 = 20(ms)$ and $f_0 = (\omega_0/2\pi) = 160Hz$.

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